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2-[((*E*)-{2-[(*E*)-(2-Hydroxybenzylidene)amino]-benzyl}imino)methyl]phenol

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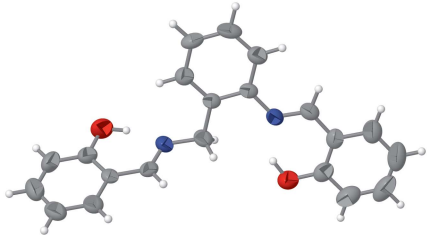
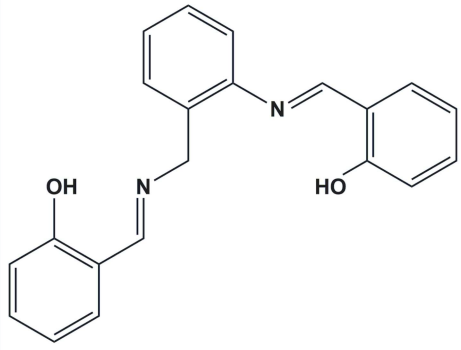
Structural data: full structural data are available from iucrdata.iucr.org

In the title hydroxyphenyl-substituted salophene compound, $C_{21}H_{18}N_2O_2$, there are two intramolecular O—H···N hydrogen bonds forming *S*(6) ring motifs. The phenol rings are inclined to one another by 65.9 (3)°, and by 0.0 (2) and 65.9 (2)°, respectively, to the central benzene ring. In the crystal, molecules are linked by a weak C—H···O contact forming chains along [010].

3D view



Chemical scheme



Structure description

The title hydroxyphenyl-substituted salophene compound was synthesized using Schiff base reactions, which play an important role in coordination chemistry (Ben Guzzi & El Alagi, 2013).

The molecular structure of the title compound is shown in Fig. 1. In the molecule, there are two intramolecular O—H···N hydrogen bonds forming *S*(6) ring motifs (Table 1 and Fig. 1). The phenol rings (C1–C6 and C16–C21) are inclined to one another by 65.9 (3)°. The C1–C6 phenol ring lies in the plane of the central benzene ring (C8–C13), with a dihedral angle of 0.0 (2)°, while the C16–C21 phenol ring is inclined to the central benzene ring (C8–C13) by 65.9 (2)°.

In the crystal, molecules are linked by weak C—H···O contacts forming chains propagating along the *b*-axis direction (Table 1 and Fig. 2).

Synthesis and crystallization

2-Aminobenzylamine (2 mmol) in methanol (50 ml) was added dropwise, with continuous stirring, to a warm methanolic solution of the appropriate salicylaldehyde (4 mmol),

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.96 (6)	1.75 (6)	2.581 (5)	142 (5)
O2—H2···N2	0.92 (5)	1.77 (5)	2.589 (5)	147 (5)
C7—H7···O2^{i}	0.93	2.63	3.526 (6)	161

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{18}N_2O_2$
M_r	330.37
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	4.8654 (14), 17.652 (6), 19.927 (6)
β (°)	91.727 (8)
V (Å^3)	1710.6 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.35 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker SMART APEXII area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.971, 0.992
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17523, 2177, 1427
R_{int}	0.069
θ_{max} (°)	22.3
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.535
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.066, 0.150, 1.16
No. of reflections	2177
No. of parameters	234
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.22

Computer programs: *APEX2* (Bruker, 2008), *SAINT* (Bruker, 2008), *SHELXS2016* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

and the mixture was refluxed for 3 h. The yellow solid obtained was filtered off, washed with cold Et_2O (10 ml) and dried in a vacuum. After a few minutes, yellow block-like crystals appeared, which were isolated *via* filtration and used without further purification.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

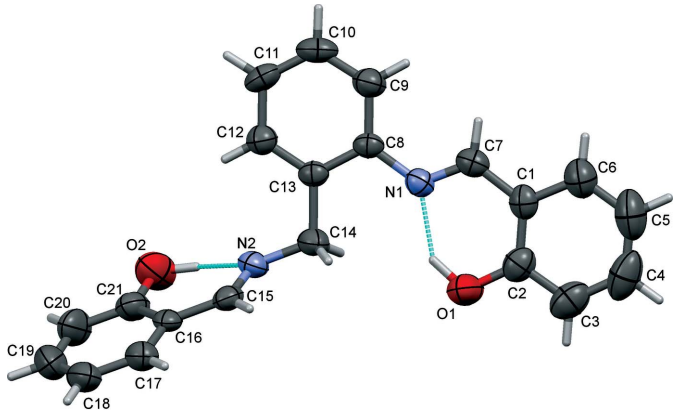


Figure 1
The molecular structure of the title compound, showing the atomic numbering and displacement ellipsoids drawn at the 30% probability level. The intramolecular O—H···N hydrogen bonds are shown as dashed lines (see Table 1).

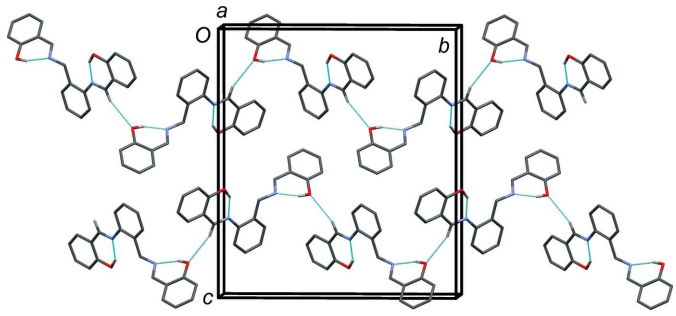


Figure 2
The crystal packing of the title compound, viewed along the *a* axis. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171209 [https://doi.org/10.1107/S2414314617012093]

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2-[((*E*)-{2-[(*E*)-(2-Hydroxybenzylidene)amino]benzyl}imino)methyl]phenol

Crystal data

$C_{21}H_{18}N_2O_2$
M_r = 330.37
Monoclinic, $P2_1/c$
a = 4.8654 (14) Å
b = 17.652 (6) Å
c = 19.927 (6) Å
β = 91.727 (8)°
V = 1710.6 (9) Å^3
Z = 4
$F(000)$ = 696
D_x = 1.283 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1427 reflections
θ = 1.5–22.3°
μ = 0.08 mm^{-1}
T = 296 K
Block, yellow
0.35 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.971, T_{max} = 0.992
17523 measured reflections
2177 independent reflections
1427 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 22.3°, θ_{min} = 2.3°
h = −5→5
k = −18→18
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.150
S = 1.16
2177 reflections
234 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0136P)^2 + 3.0321P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.0311 (9)	0.4754 (2)	0.09631 (18)	0.0762 (11)
H1	0.112 (12)	0.455 (3)	0.126 (3)	0.11 (2)*
O2	0.7654 (10)	0.1330 (2)	0.12620 (19)	0.0856 (13)
H2	0.656 (11)	0.175 (3)	0.131 (3)	0.09 (2)*
N1	0.2561 (7)	0.4637 (2)	0.20684 (17)	0.0440 (9)
N2	0.6237 (8)	0.2743 (2)	0.12028 (18)	0.0491 (10)
C1	−0.0757 (9)	0.5601 (2)	0.1879 (2)	0.0489 (12)
C2	−0.1524 (10)	0.5363 (3)	0.1230 (3)	0.0572 (13)
C3	−0.3537 (11)	0.5745 (3)	0.0867 (3)	0.0766 (16)
H3	−0.402875	0.558447	0.043505	0.092*
C4	−0.4815 (12)	0.6357 (4)	0.1136 (4)	0.088 (2)
H4	−0.618823	0.660737	0.088810	0.105*
C5	−0.4099 (13)	0.6606 (3)	0.1764 (4)	0.090 (2)
H5	−0.495865	0.702795	0.194215	0.108*
C6	−0.2102 (11)	0.6230 (3)	0.2133 (3)	0.0696 (15)
H6	−0.163483	0.640004	0.256330	0.084*
C7	0.1301 (9)	0.5220 (3)	0.2282 (2)	0.0476 (12)
H7	0.173152	0.540229	0.270990	0.057*
C8	0.4603 (8)	0.4252 (2)	0.2448 (2)	0.0398 (11)
C9	0.5489 (10)	0.4456 (3)	0.3096 (2)	0.0551 (13)
H9	0.471246	0.487282	0.330369	0.066*
C10	0.7494 (10)	0.4046 (3)	0.3429 (2)	0.0575 (13)
H10	0.804140	0.418456	0.386321	0.069*
C11	0.8712 (9)	0.3433 (3)	0.3133 (2)	0.0544 (13)
H11	1.008338	0.315912	0.335980	0.065*
C12	0.7847 (9)	0.3234 (3)	0.2490 (2)	0.0503 (12)
H12	0.866455	0.282191	0.228447	0.060*
C13	0.5812 (8)	0.3627 (2)	0.2145 (2)	0.0392 (11)
C14	0.4834 (9)	0.3410 (3)	0.1441 (2)	0.0529 (13)
H14	0.287088	0.331458	0.143787	0.063*
H13	0.515840	0.382958	0.113827	0.063*
C15	0.7827 (9)	0.2816 (2)	0.0713 (2)	0.0468 (12)
H15	0.798118	0.328849	0.050982	0.056*
C16	0.9399 (9)	0.2192 (2)	0.0461 (2)	0.0425 (11)
C17	1.1157 (10)	0.2311 (3)	−0.0068 (2)	0.0569 (13)
H17	1.125123	0.278977	−0.026086	0.068*
C18	1.2748 (11)	0.1740 (4)	−0.0312 (3)	0.0718 (16)
H18	1.390668	0.182823	−0.066642	0.086*
C19	1.2609 (13)	0.1040 (4)	−0.0028 (3)	0.0872 (19)
H19	1.368830	0.065028	−0.019071	0.105*
C20	1.0912 (14)	0.0900 (3)	0.0493 (3)	0.0870 (19)
H20	1.084064	0.041860	0.068086	0.104*
C21	0.9311 (11)	0.1473 (3)	0.0738 (2)	0.0612 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.100 (3)	0.074 (3)	0.053 (2)	0.018 (2)	−0.012 (2)	−0.005 (2)
O2	0.133 (4)	0.061 (3)	0.064 (3)	0.012 (3)	0.013 (3)	0.016 (2)
N1	0.050 (2)	0.043 (2)	0.039 (2)	0.0002 (19)	0.0056 (18)	−0.0015 (18)
N2	0.061 (3)	0.049 (2)	0.037 (2)	0.004 (2)	−0.001 (2)	−0.0075 (18)
C1	0.044 (3)	0.044 (3)	0.059 (3)	0.000 (2)	0.010 (2)	0.005 (2)
C2	0.059 (3)	0.052 (3)	0.061 (4)	−0.002 (3)	0.000 (3)	0.013 (3)
C3	0.079 (4)	0.076 (4)	0.074 (4)	−0.004 (3)	−0.010 (3)	0.022 (3)
C4	0.067 (4)	0.078 (5)	0.119 (6)	0.010 (4)	0.003 (4)	0.044 (4)
C5	0.079 (5)	0.064 (4)	0.127 (6)	0.019 (3)	0.023 (4)	0.007 (4)
C6	0.068 (4)	0.062 (4)	0.079 (4)	0.009 (3)	0.009 (3)	0.000 (3)
C7	0.053 (3)	0.049 (3)	0.041 (3)	−0.006 (2)	0.005 (2)	−0.004 (2)
C8	0.043 (3)	0.044 (3)	0.032 (3)	−0.006 (2)	0.003 (2)	0.001 (2)
C9	0.067 (3)	0.055 (3)	0.044 (3)	0.001 (3)	0.001 (3)	−0.004 (2)
C10	0.074 (4)	0.066 (3)	0.032 (3)	−0.020 (3)	−0.003 (3)	−0.002 (3)
C11	0.056 (3)	0.064 (3)	0.042 (3)	−0.004 (3)	−0.013 (2)	0.013 (3)
C12	0.053 (3)	0.051 (3)	0.047 (3)	0.001 (2)	−0.002 (2)	−0.001 (2)
C13	0.041 (3)	0.043 (3)	0.034 (2)	−0.005 (2)	0.002 (2)	0.002 (2)
C14	0.053 (3)	0.063 (3)	0.042 (3)	0.004 (2)	−0.004 (2)	−0.010 (2)
C15	0.056 (3)	0.046 (3)	0.037 (3)	0.002 (2)	−0.012 (2)	0.001 (2)
C16	0.051 (3)	0.045 (3)	0.030 (3)	0.002 (2)	−0.009 (2)	−0.008 (2)
C17	0.060 (3)	0.064 (3)	0.046 (3)	0.005 (3)	−0.003 (3)	−0.005 (3)
C18	0.069 (4)	0.099 (5)	0.047 (3)	0.017 (4)	−0.002 (3)	−0.011 (3)
C19	0.098 (5)	0.094 (5)	0.069 (4)	0.040 (4)	−0.009 (4)	−0.025 (4)
C20	0.131 (6)	0.058 (4)	0.071 (4)	0.038 (4)	−0.012 (4)	0.005 (3)
C21	0.085 (4)	0.055 (3)	0.043 (3)	0.010 (3)	−0.008 (3)	0.001 (3)

Geometric parameters (Å, º)

O1—C2	1.344 (6)	C9—H9	0.9300
O1—H1	0.96 (6)	C10—C11	1.375 (6)
O2—C21	1.362 (6)	C10—H10	0.9300
O2—H2	0.92 (5)	C11—C12	1.382 (6)
N1—C7	1.278 (5)	C11—H11	0.9300
N1—C8	1.405 (5)	C12—C13	1.376 (6)
N2—C15	1.271 (5)	C12—H12	0.9300
N2—C14	1.448 (5)	C13—C14	1.518 (5)
C1—C6	1.393 (6)	C14—H14	0.9700
C1—C2	1.398 (6)	C14—H13	0.9700
C1—C7	1.432 (6)	C15—C16	1.440 (6)
C2—C3	1.377 (7)	C15—H15	0.9300
C3—C4	1.365 (8)	C16—C21	1.385 (6)
C3—H3	0.9300	C16—C17	1.394 (6)
C4—C5	1.362 (8)	C17—C18	1.369 (7)
C4—H4	0.9300	C17—H17	0.9300
C5—C6	1.371 (8)	C18—C19	1.361 (8)

C5—H5	0.9300	C18—H18	0.9300
C6—H6	0.9300	C19—C20	1.368 (8)
C7—H7	0.9300	C19—H19	0.9300
C8—C13	1.397 (6)	C20—C21	1.375 (7)
C8—C9	1.397 (6)	C20—H20	0.9300
C9—C10	1.370 (6)		

C2—O1—H1	112 (3)	C10—C11—H11	120.8
C21—O2—H2	107 (3)	C12—C11—H11	120.8
C7—N1—C8	123.3 (4)	C13—C12—C11	122.0 (4)
C15—N2—C14	118.2 (4)	C13—C12—H12	119.0
C6—C1—C2	117.4 (5)	C11—C12—H12	119.0
C6—C1—C7	119.9 (5)	C12—C13—C8	119.3 (4)
C2—C1—C7	122.7 (4)	C12—C13—C14	122.4 (4)
O1—C2—C3	119.8 (5)	C8—C13—C14	118.3 (4)
O1—C2—C1	119.9 (4)	N2—C14—C13	111.7 (4)
C3—C2—C1	120.3 (5)	N2—C14—H14	109.3
C4—C3—C2	120.4 (6)	C13—C14—H14	109.3
C4—C3—H3	119.8	N2—C14—H13	109.3
C2—C3—H3	119.8	C13—C14—H13	109.3
C5—C4—C3	120.6 (6)	H14—C14—H13	107.9
C5—C4—H4	119.7	N2—C15—C16	122.1 (4)
C3—C4—H4	119.7	N2—C15—H15	118.9
C4—C5—C6	119.6 (6)	C16—C15—H15	118.9
C4—C5—H5	120.2	C21—C16—C17	117.8 (4)
C6—C5—H5	120.2	C21—C16—C15	122.7 (4)
C5—C6—C1	121.6 (6)	C17—C16—C15	119.5 (4)
C5—C6—H6	119.2	C18—C17—C16	121.6 (5)
C1—C6—H6	119.2	C18—C17—H17	119.2
N1—C7—C1	121.7 (4)	C16—C17—H17	119.2
N1—C7—H7	119.1	C19—C18—C17	119.0 (5)
C1—C7—H7	119.1	C19—C18—H18	120.5
C13—C8—C9	118.7 (4)	C17—C18—H18	120.5
C13—C8—N1	116.7 (4)	C18—C19—C20	121.2 (5)
C9—C8—N1	124.6 (4)	C18—C19—H19	119.4
C10—C9—C8	120.5 (4)	C20—C19—H19	119.4
C10—C9—H9	119.7	C19—C20—C21	119.8 (5)
C8—C9—H9	119.7	C19—C20—H20	120.1
C9—C10—C11	121.2 (4)	C21—C20—H20	120.1
C9—C10—H10	119.4	O2—C21—C20	119.4 (5)
C11—C10—H10	119.4	O2—C21—C16	120.1 (4)
C10—C11—C12	118.3 (4)	C20—C21—C16	120.5 (5)

C6—C1—C2—O1	−179.3 (4)	C11—C12—C13—C14	−179.6 (4)
C7—C1—C2—O1	0.0 (7)	C9—C8—C13—C12	−0.5 (6)
C6—C1—C2—C3	0.0 (7)	N1—C8—C13—C12	179.2 (4)
C7—C1—C2—C3	179.3 (4)	C9—C8—C13—C14	180.0 (4)
O1—C2—C3—C4	179.0 (5)	N1—C8—C13—C14	−0.3 (5)

C1—C2—C3—C4	−0.3 (8)	C15—N2—C14—C13	−113.7 (4)
C2—C3—C4—C5	0.8 (9)	C12—C13—C14—N2	1.7 (6)
C3—C4—C5—C6	−0.9 (9)	C8—C13—C14—N2	−178.7 (4)
C4—C5—C6—C1	0.6 (9)	C14—N2—C15—C16	177.3 (4)
C2—C1—C6—C5	−0.1 (7)	N2—C15—C16—C21	−0.7 (7)
C7—C1—C6—C5	−179.5 (5)	N2—C15—C16—C17	−178.6 (4)
C8—N1—C7—C1	179.6 (4)	C21—C16—C17—C18	0.2 (7)
C6—C1—C7—N1	179.3 (4)	C15—C16—C17—C18	178.2 (4)
C2—C1—C7—N1	0.0 (7)	C16—C17—C18—C19	−0.2 (8)
C7—N1—C8—C13	−179.5 (4)	C17—C18—C19—C20	0.1 (9)
C7—N1—C8—C9	0.2 (6)	C18—C19—C20—C21	−0.1 (9)
C13—C8—C9—C10	−0.4 (6)	C19—C20—C21—O2	−179.2 (5)
N1—C8—C9—C10	179.9 (4)	C19—C20—C21—C16	0.1 (8)
C8—C9—C10—C11	0.9 (7)	C17—C16—C21—O2	179.1 (4)
C9—C10—C11—C12	−0.6 (7)	C15—C16—C21—O2	1.2 (7)
C10—C11—C12—C13	−0.4 (7)	C17—C16—C21—C20	−0.1 (7)
C11—C12—C13—C8	0.9 (6)	C15—C16—C21—C20	−178.1 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.96 (6)	1.75 (6)	2.581 (5)	142 (5)
O2—H2···N2	0.92 (5)	1.77 (5)	2.589 (5)	147 (5)
C7—H7···O2^{i}	0.93	2.63	3.526 (6)	161

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+1/2.